

Chaos in coplanar classical collisions with particles interacting through r^{-2} forces

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The scattering among three particles interacting through $1/r^2$ forces, with opposite charges and widely different masses, is studied in a coplanar geometry. The present work shows that at low impact velocities the output of the collision presents typical fingerprints of chaos. The details of the process are investigated.

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Starting from the works of Gaspard and Rice [1], chaotic scattering was found to be ubiquitous. A large amount of work has been done on potential scattering (*i.e.* scattering of an elementary particle on fixed potential centers) [2–5], but also the scattering among at least three interacting bodies has received great attention (see the work of Petit and Hénon on the scattering between a planet and two satellites [6], or the system helium nucleus plus two electrons [7]). A monographic issue about this subject has been published in the journal CHAOS [8].

In all these studies the projectile and a target preserve their internal structure during the collision, but one can analyze also reactive collisions. Kovács and Wiesenfeld [9] studied, in a collinear geometry, the scattering between an atom and a diatomic molecule: $A + BC \leftrightarrow ABC \leftrightarrow AB + C$. More recently, we studied the chaotic behavior in the reaction between a hydrogen atom (proton plus electron) and a projectile proton interacting through Coulomb forces [10]. We analyzed the full three-dimensional problem at very low impact energies. We found that the transition from regular to chaotic scattering appears when impact velocity v_p is reduced to a value below about 1/10 of the classical electron velocity v_e .

In this paper we present another investigation on the same subject: we think that it is worth consideration since collisions with rearrangement between electrically charged particles are one current topic in atomic physics, both on the theoretical as well the experimental side [11]. The phase space of a system of three particles moving in 3D is too large to be easily handled; limiting to 2D will allow us to do a more detailed and accurate study. We will address the following topics: a) Do features of chaotic scattering appear in two-dimensional collisions? b) If so, do they appear in the form of a sharp order–chaos transition, or as a smooth transition? c) Is it possible to detect some traces of irregular behaviour also in the heavy particles motion, instead that only when looking at the lightest one? d) Finally, an investigation of the dynamics of the electron during the scattering is done. It gives an insight on how the discontinuities on the output function appear.

The final state of the projectile may be defined through a set of parameters $\{A_f\}$ (*e.g.* angle of deflection, final velocity, ...), which are functions of the input quantities $\{A_i\}$ (*e.g.* impact parameter, impact velocity, ...). When the set of values $\{A_f\}$ depends sensitively by $\{A_i\}$, *i.e.* a finite variation of $\{A_f\}$ is caused by an infinitesimal variation of $\{A_i\}$, then the system is chaotic.

Usually, one studies the so-called *scattering functions*, which are the output variables as a function of only one input variable, keeping the other input variables fixed. If a scattering function is fractal then the system is chaotic but the converse is not necessarily true. In fact, Chen *et al.* [12] showed that time-independent Hamiltonian systems with more than two degrees of freedom can have chaotic sets with nonzero fractal dimension while at the same time the scattering functions do not show any fractal property. The scattering function has fractal behaviour only if the Hausdorff dimension D_c of the chaotic invariant set satisfies the inequality

$$D_c > 2N - (2 + q) \quad (1)$$

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where N is the number of degrees of freedom and q is the number of conserved quantities of the system (in our case $N = 6$ and $q = 4$). Therefore a positive answer to the above question (a) will give us also a lower bound estimate of the Hausdorff dimension of the chaotic set of the system.

Our scattering problem has the following alternative outcomes:

$$H + H^+ \rightarrow H^+ + H \quad (2)$$

$$\rightarrow e + H^+ + H^+ \quad (3)$$

$$\rightarrow H + H^+ \quad (4)$$

At the end of the collision the electron may be captured by the projectile nucleus (charge transfer), may be ionized (ionization), or may remain bound to the target (excitation of the target). The values of the masses and charges are $m_{H^+} = 1836$, $m_e \equiv 1836$, $Q_e = -Q_{H^+} = -1$ (atomic units will be used throughout this paper).

In our geometry the scattering plane is the plane (x, y) . The target proton is initially fixed at the origin, $\mathbf{r}_t = (0, 0)$, and at rest, $\mathbf{v}_t = (0, 0)$. The position of the electron is $\mathbf{r}_e = (r_e \cos \theta + \omega_e t, r_e \sin \theta + \omega_e t)$, where r_e is the radius, θ is the initial phase, $\omega_e = v_e/r_e$ is the angular velocity. Both v_e and r_e are equal to 1 in our units. The projectile proton is prepared with velocity v_p in the positive direction of the y -axis and at the position $\mathbf{r}_p = (b, -a)$, where b is the impact parameter and $a > 0$ must be chosen so large that the target and the projectile may be considered initially as non-interacting. In these simulations $a \simeq 10$ was found to be a good choice.

The total energy of the system is given by

$$E = \frac{1}{2}m_{H^+}v_t^2 + \frac{1}{2}m_{H^+}v_p^2 + \frac{1}{2}m_e v_e^2 + \frac{1}{|\mathbf{r}_t - \mathbf{r}_p|} - \frac{1}{|\mathbf{r}_t - \mathbf{r}_e|} - \frac{1}{|\mathbf{r}_p - \mathbf{r}_e|} \quad (5)$$

The classical equations of motion are numerically integrated by using a variable-order variable-step Adams algorithm (routine NAG D02CJF).

Please, note that the choice of the outcome is done on the basis of the energy of the electron with respect to the two bodies. An algorithm to identify all the possible outcomes is given in ref. [13]. In particular, in our system three parameters remain free: θ , v_p , and b . Numerical simulations have been carried out varying all of them. The output variables $\{A_f\}$ defined above reduce to just one element—the final state of the electron. It is a discrete function of its energy. Discrete variables are usually not employed in these studies but are not a novelty: already Bleher *et al* [14] investigated a chaotic system with a finite number of possible outcomes.

In Figures 1 and 2 some consecutive blow-ups of the scattering function are presented as a function of b , for two different choices of v_p and θ . There are regions where the outcome is a regular function of b , alternated with other regions where an irregular behaviour appears. One recognizes a kind of self similarity, the same pattern repeating at smaller and smaller scales. This is the distinctive aspect of fractal behaviour. The same results appear varying θ , at v_p and b fixed.

A clear picture is obtained by studying the scattering function *versus* the proton velocity v_p . In Figure 3 this is shown for one couple of values (b, θ) . It is visible the great degree of irregularity at small v_p 's. For higher v_p 's the zones where the electron is captured and those where it remains close to the target proton are more clear-cut. Ionization is by far the least probable process. One may judge that the transition order-chaos does appear quite smooth and the scattering at $v \simeq 0.2, 0.3$ is not yet entirely regular.

In order to quantify the amount of chaos one can compute the fractal dimension of the scattering function. Given a reference trajectory with initial impact parameter b , we slightly modify the impact parameter to $b + \epsilon$ and make another run. The results of the two runs are compared. The starting trajectory is said uncertain if the two final states are different. The fraction $f(\epsilon)$ of uncertain trajectories as a function of the parameter ϵ scales as

$$f(\epsilon) \sim \epsilon^{1-d}, \quad \text{for } \epsilon \rightarrow 0, \quad (6)$$

where d is the capacity dimension [3]. In Figure 4 we plot the capacity dimension d as a function of v_p . There is a regular decrease of d for $v_p < 0.3$, then d is nearly constant but positive.

One of the main purposes of this work is to analyze in detail the behaviour of the electron in correspondence of a singularity of the scattering function. In Figure 5 the trajectories of the particles are shown for two almost identical runs, differing only by a very small value of the impact parameter. We see that initially the electron trajectories in the two cases nearly overlap. The two paths begin to differ when the nuclei reach the point of closest approach. The potential felt by the electron may be sketched as two wells located around the nuclei divided by a symmetrical ridge. Obviously, the location of the ridge dynamically evolves in time as the nuclei move. The electron initially lies in

one of the two potential wells and it is able to escape to the other well only if at some time during the collision it passes near the ridge with enough velocity to cross it. Note that we are referring to the component of the velocity orthogonal to the potential ridge. Once the electron has fallen into the other potential well it is very unlikely that it can cross the ridge the opposite way and come back to the former nucleus. Two electrons differing by an infinitesimal value of the velocity, $u, u + \epsilon$ will undergo entirely different fates provided that $u + \epsilon$ is not enough to cross the potential barrier while u is.

It is interesting to notice that chaotic features appear only as singularities of the scattering function: An analysis of the delay time (the time needed by the electron to quit the interaction region) reveals that it is not a sensitive function of the scattering. This is related to the fact that the electron does closely follow one of the nuclei, and the trajectories of the heavy particles are always regular: no complicated patterns appear from a study of their behaviour.

In summary, a study of the two-dimensional low energy scattering between charged particles has been carried out. Simulations have been done using a larger number of runs than in our previous paper [10] so diminishing statistical errors. The results confirm the findings of ref. [10] that the scattering becomes irregular when the energy is low enough. An insight on why chaos appears has been given by looking at the detailed trajectories of the electron. Abrupt discontinuities in the output function are correlated with the structure of the potential seen by the electron.

It is useful to spend some words about the validity of the model used. At very small impact velocities, it is not entirely justified to treat the heavy particles as classical objects, and even less the light particle. The processes (2-4) should be studied within the framework of quantum mechanics. However: i) one may imagine to apply the same apparatus not to the ground state but to a Rydberg state, where using the classical mechanics is justified; ii) the use of classical or semiclassical models has recently been extended with satisfactory results in realms thought previously to be amenable only to quantum treatment, see for example the classical description of the helium atom [15], or the treatment of the hydrogen ionization by electron scattering at energies near threshold [16]. In that work, furthermore, the evidence for chaos was found, reminiscent of the results shown in this paper.

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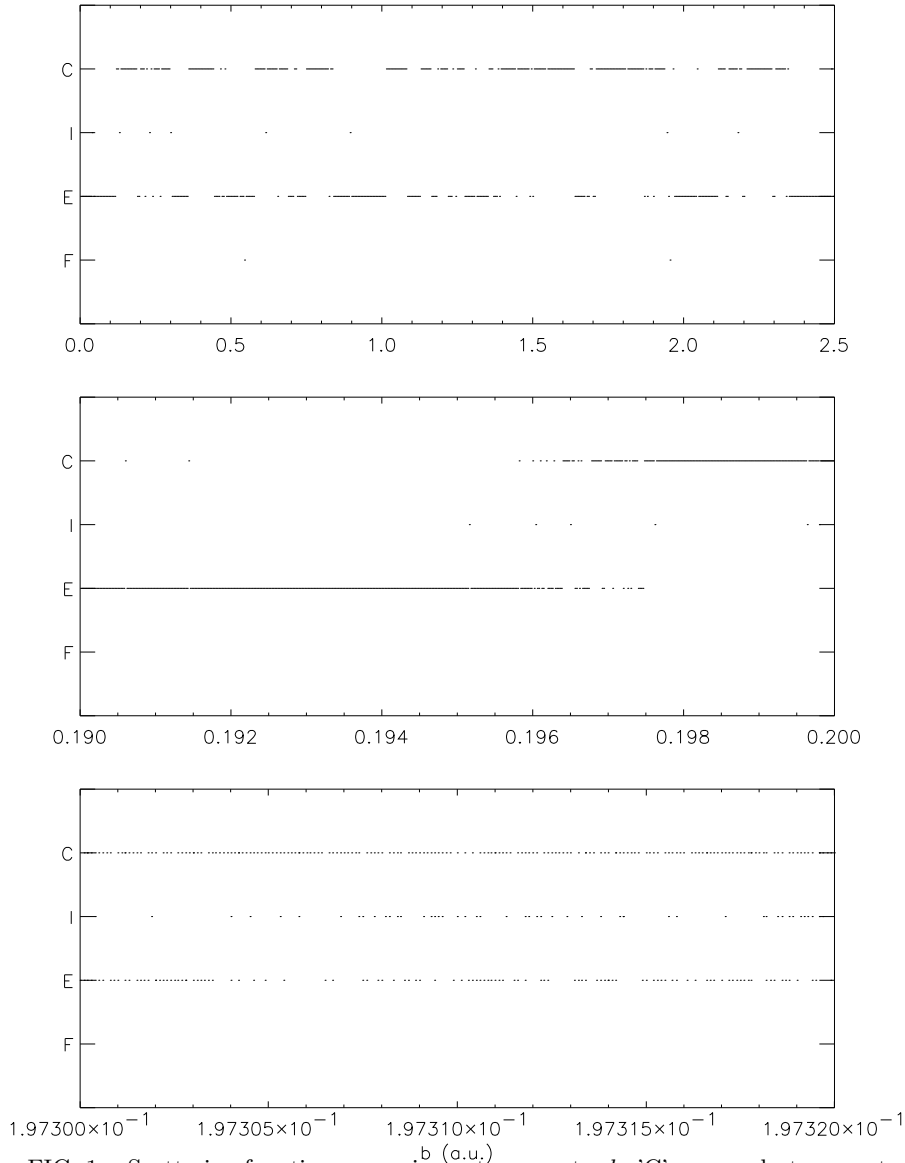


FIG. 1. Scattering function *versus* impact parameter b . 'C' means electron capture; 'I', ionization; 'E', electronic excitation; 'F', undetermined. Here $v = 0.10$, $\theta = 5.82512$ radians. From top to bottom successive enlargements are shown with respect to b . The number of runs is about 500 for each plot.

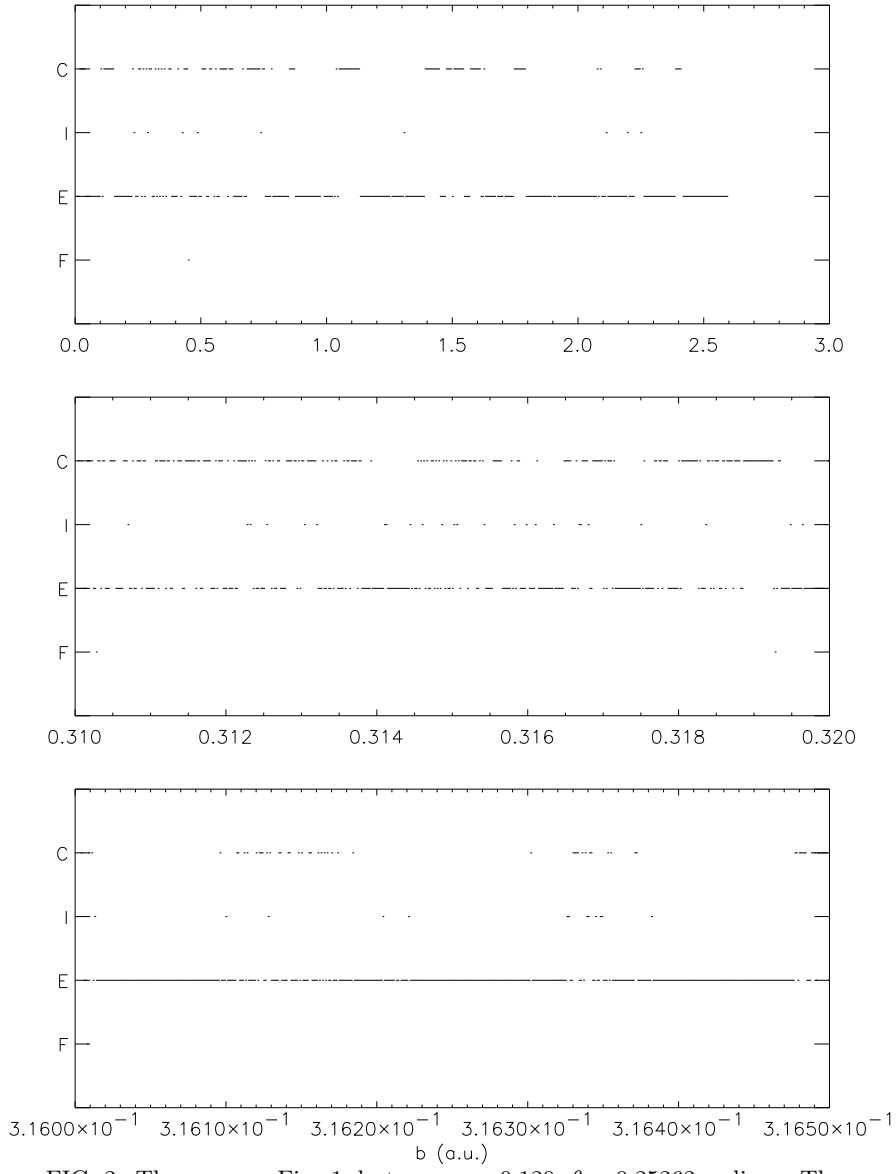


FIG. 2. The same as Fig. 1, but now $v = 0.120$, $\theta = 0.25262$ radians. The number of runs is about 500 for each plot.

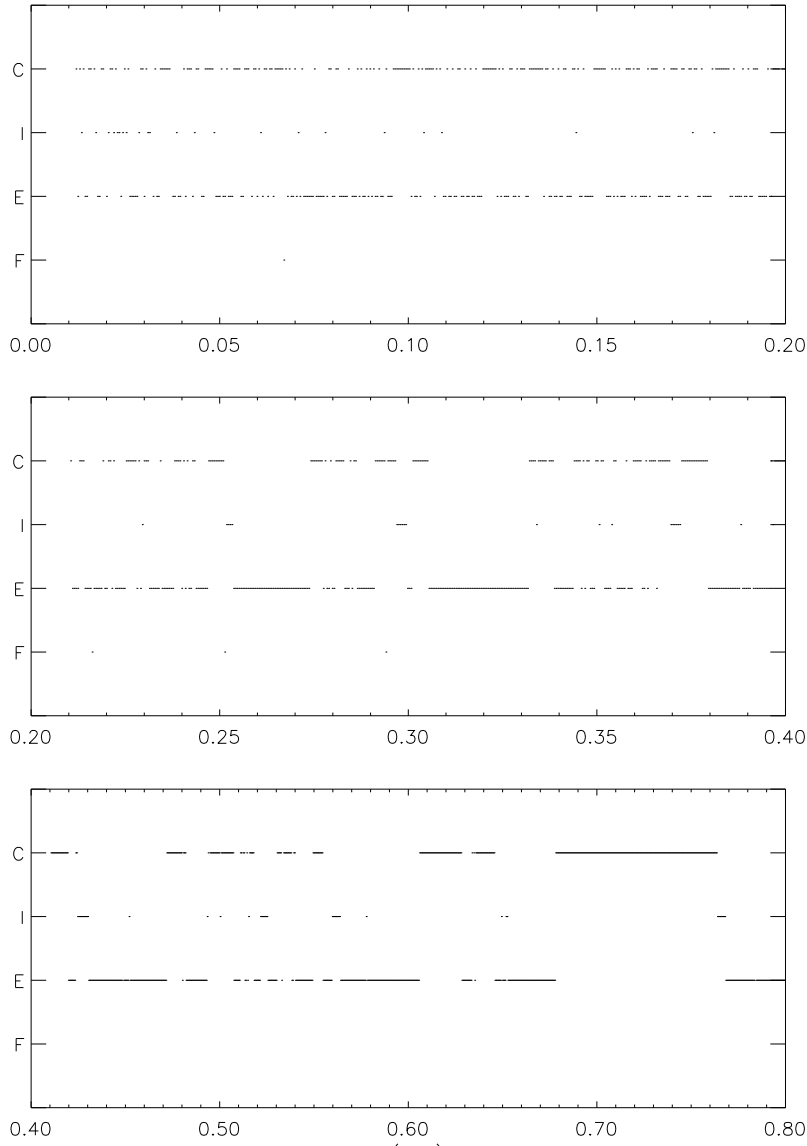


FIG. 3. Scattering function *versus* impact velocity v . $b = 0.2893$, $\theta = 5.82512$ radians. The number of runs is about 400 for each plot.

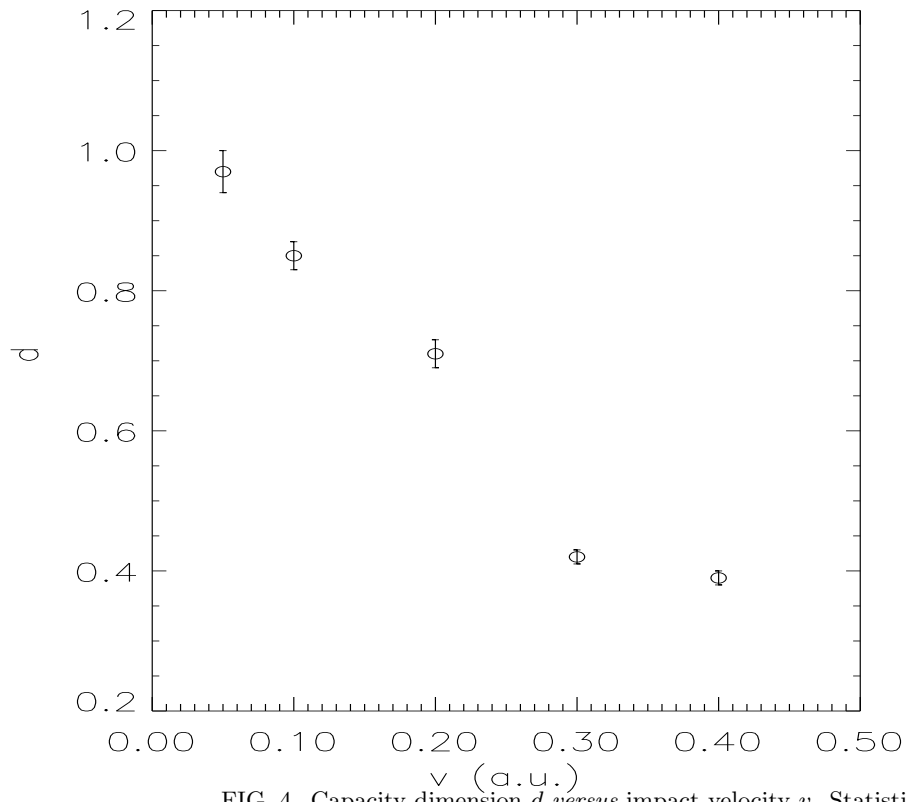


FIG. 4. Capacity dimension d *versus* impact velocity v . Statistical errors are shown.

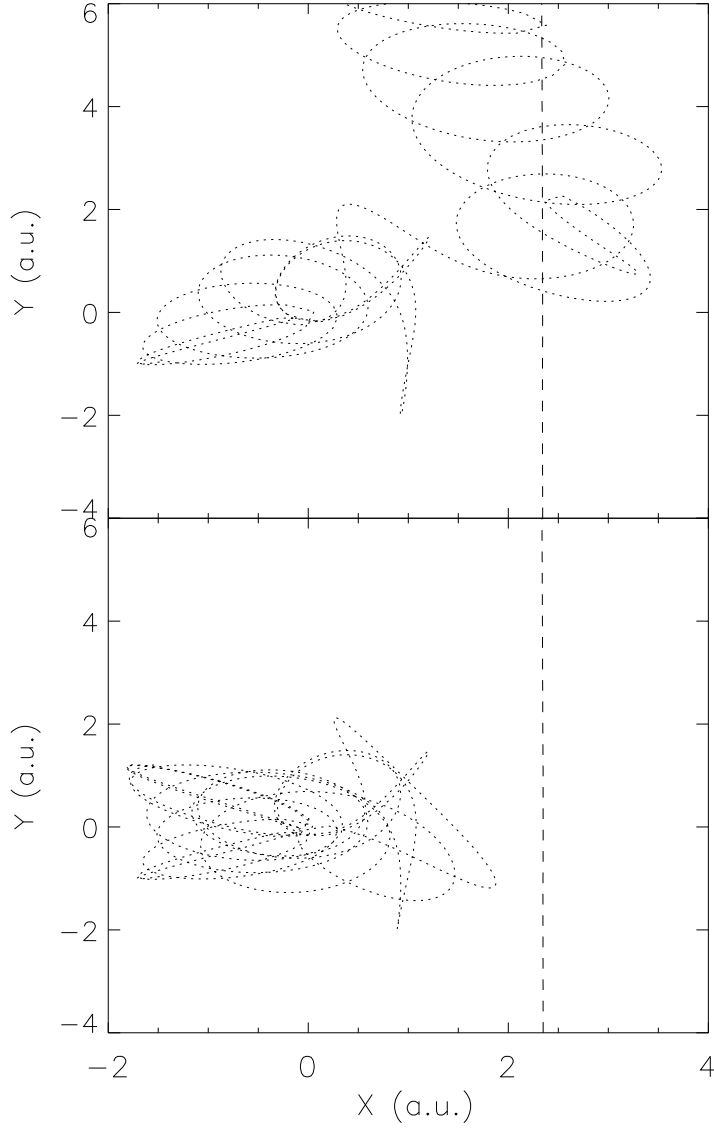


FIG. 5. Upper, trajectories of the particles in the interaction region. $v = 0.10$, $\theta = 5.82512$ radians, and $b = 2.345$. The dashed line is the trajectory of the heavy projectile. The electron trajectory is the dotted line. The initial position of the electron is close to $(0, 0)$. The trajectory of the target nucleus is not shown since it is always close to the origin $(0, 0)$. The lower panel shows the same process, but now with $b = 2.350$.